TOPS Meeting

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Lawrence Livermore National Laboratory

Report on TAO and Multigrid Methods for Optimization

http://www.mcs.anl.gov/lans

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Research Participants

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- PETSc developing team
- PDE/Optimization seminar participants

Outline

- TAO
  - Introduction
  - New developments and future plans
- Multigrid Methods
  - Optimal control problem
  - Benchmark problems
  - Grid sequencing - preliminary results

TAO

Definition (Webster) Chinese (Beijing) dào, 1736.

1. The process of nature by which all things change and which is to be followed for a life of harmony.
2. Toolkit for advanced optimization

Mantra

Design and implementation of algorithms and component-based software for the solution of large-scale optimization applications on high-performance architectures.

- Component-based interaction
- Leverage of existing parallel computing infrastructure
- Reuse of external (preconditioners, linear solvers . . .) toolkits

TAO: New Developments and Future Plans

New Developments

- ◇ Release of Version 1.3
- ◇ ESI interface (compliance with Trilinos)
- ◇ Development of BLMVM
- ◇ Nonlinear complementarity solvers
- ◇ TAO/CCA demo at SC2000 (www.mcs.anl.gov/cca/cca_demos.html)

Future Plans

- ◇ Nonlinear least squares solvers
- ◇ Integration of TAO into MPQC and NWChem
- ◇ Use of automatic differentiation tools (ADIC) in TAO

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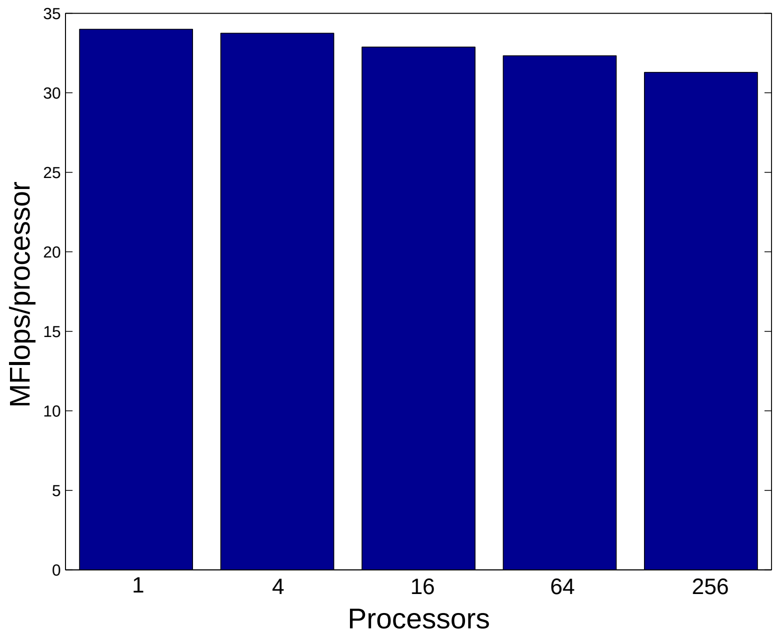
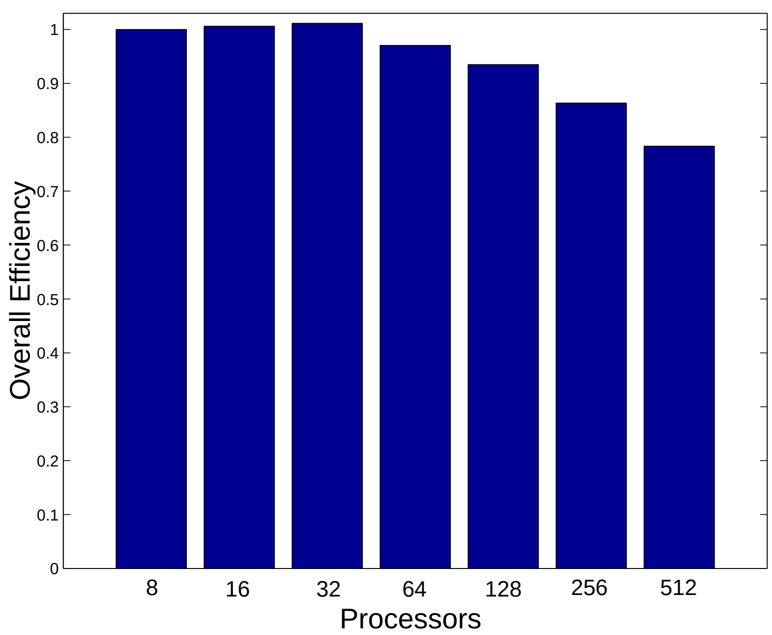
TAO Performance of BLMVM: Plate Problem

Cray T3E (NERSC)

$n = 2.56 \cdot 10^6$ variables





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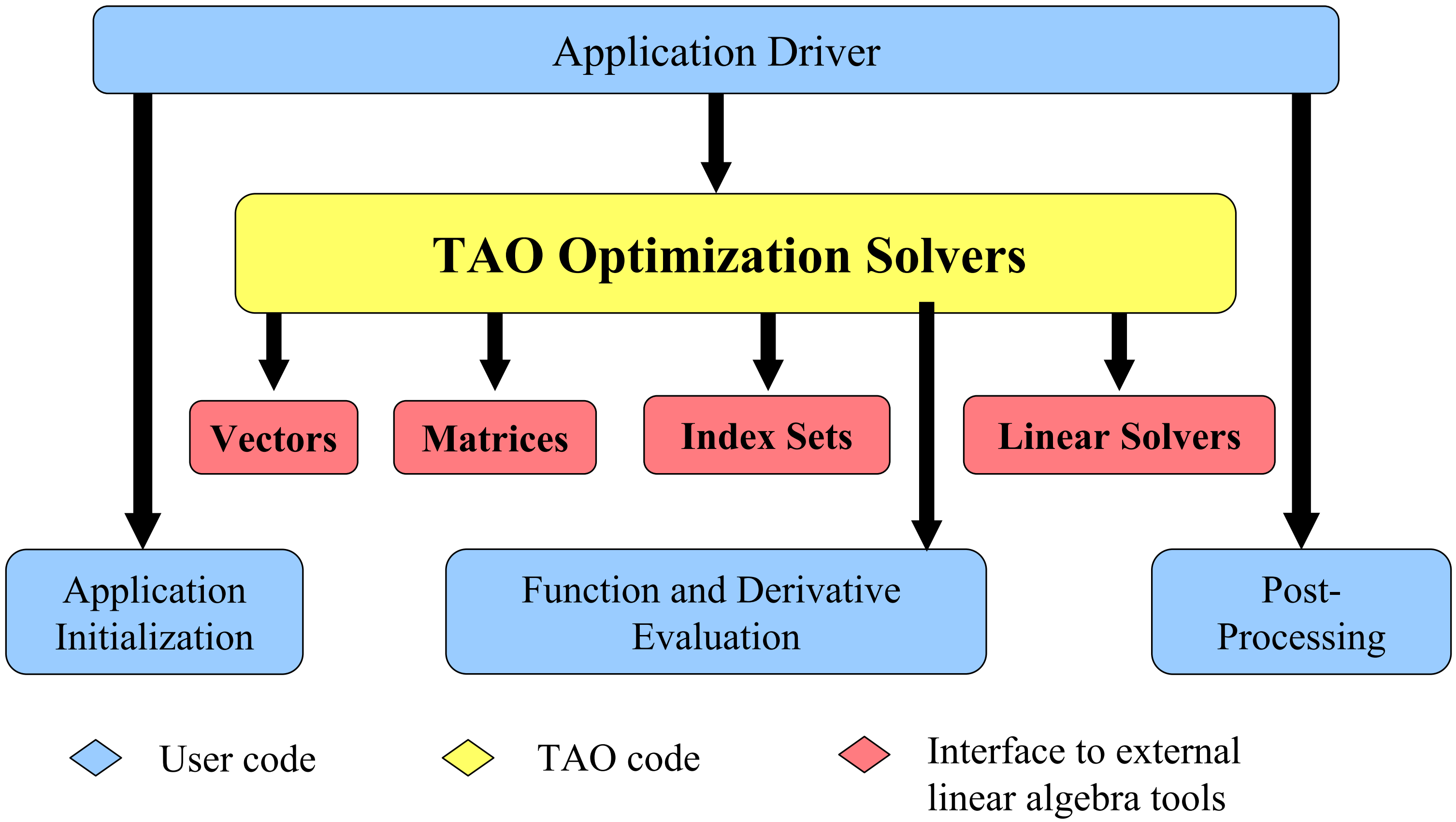
TAO: CCA Interactions



TAO

www.mcs.anl.gov/tao

Version 1.3 (December 2001)

- Source Code
- Documentation
- Installation instructions
- Tutorials (NERSC, September 2000)
- Example problems
- Performance results
- Supported architectures

Optimal Control Problems

The optimal control problem requires minimizing

$$f_c[t_l, x(t_l), t_u, x(t_u)]$$

subject to the state equations,

$$x'(t) = f[t, x(t), u(t)], \qquad t \in [t_l, t_u],$$

boundary conditions on the states, and the control constraints,

$$u(t) \in U, \qquad t \in [t_l, t_u].$$

Note. The solution is bang-bang if for some interval I,

$$u(t) \in \partial U, \qquad t \in I$$

The COPS Benchmarks

COPS has optimal control and parameter estimation problems, with descriptions of the formulations as optimization problems and numerical results for several optimization solvers.

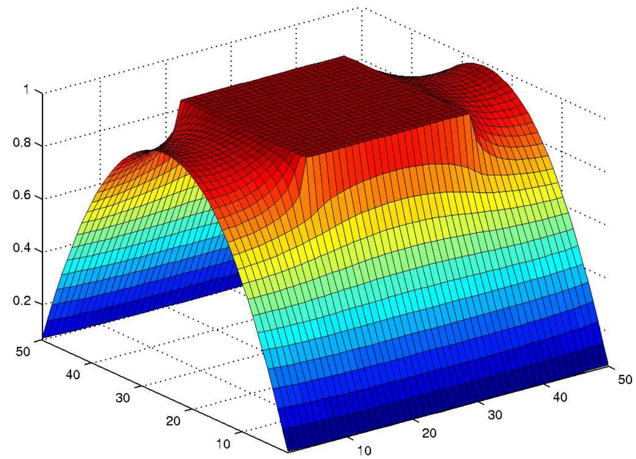
- Robot arm
- Particle steering
- Goddard rocket
- Hang glider
- Marine population dynamics
- Flow in a channel
- Methanol to hydrocarbons
- Isomerization of α-pinene

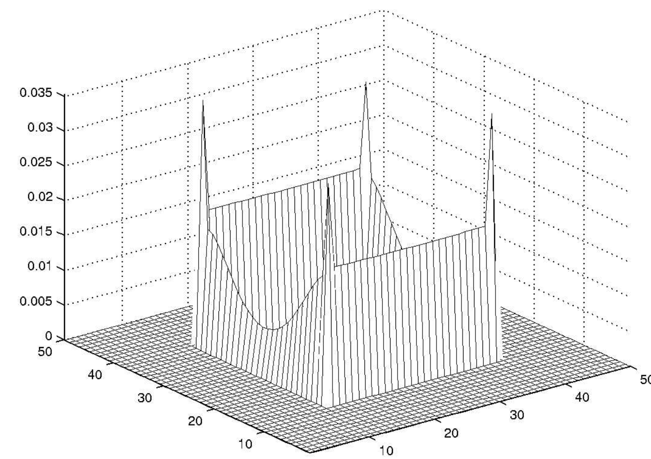
Optimal Control: Computational Issues

- The optimization approach is relatively recent
- The optimization approach overcomes many of the difficulties from the Pontryagin maximum principle
- The optimization approach applies to sliding and chattering controls.
- Algorithms have a wide range in performance possibly due to the lack of good initial guesses.
- The number of iterations of current optimization algorithms is mesh dependent.
- Techniques for dealing with the lack of smoothness in the state and the control are ad-hoc.

Example: Minimal Surface with Obstacles

Number of active constraints depends on the height of the obstacle. The solution $v \notin C^1$. Almost all multipliers are zero.





Note. See Bank, Gill, and Marcia (2001) for numerical results with an interior point method.

Benchmark Problems

- Variational problems with bounds on the control
- Convex problems
- Unique solutions
- Five different problems
- Three different choices of parameters per problem
- Cost per variable is constant
- Target problems with 10^5 variables

Goal. Develop algorithms with bounded cost per grid point

Grid Sequencing Issues

- ◇ How much does grid-sequencing save?
- ◇ Does grid-sequencing resolve the convergence issue?
- ◇ What is the order of convergence of $f(x_h^*)$?
- ◇ What is the order of convergence of x_h^*?
- ◇ How does the number of active constraints at x_h change?
- ◇ What tolerance do we use to obtain x_h?
- ◇ What is the impact on iterative methods on these results?

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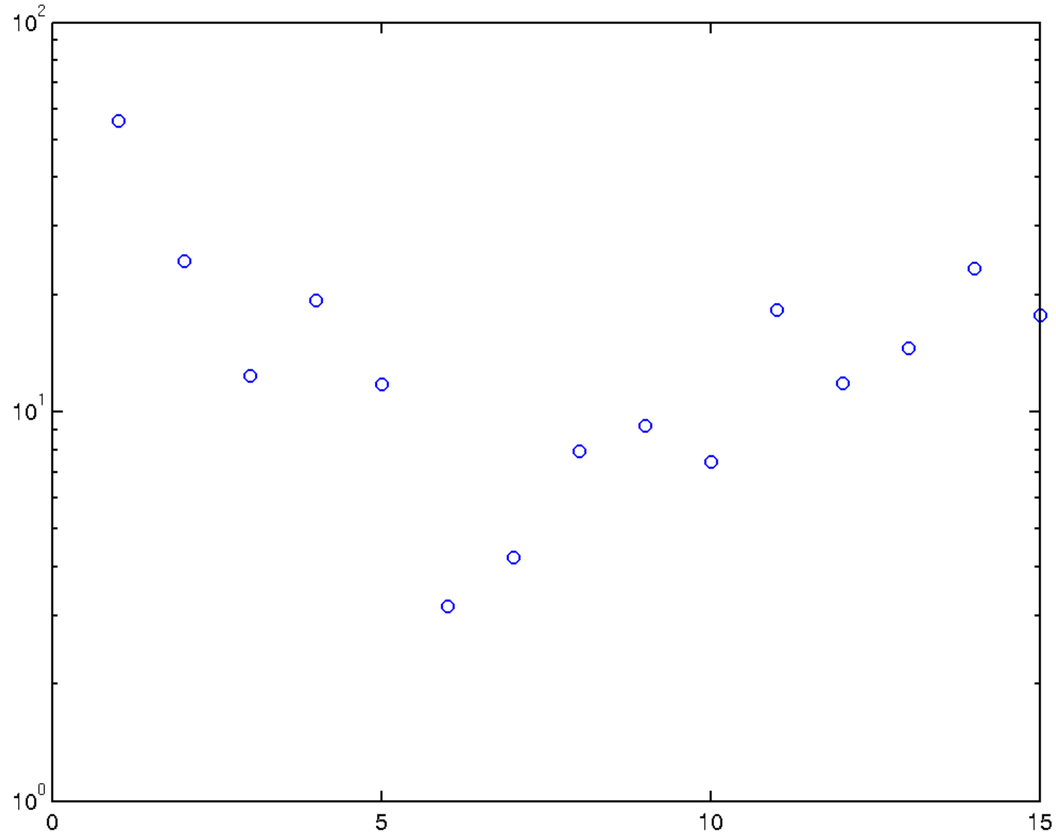
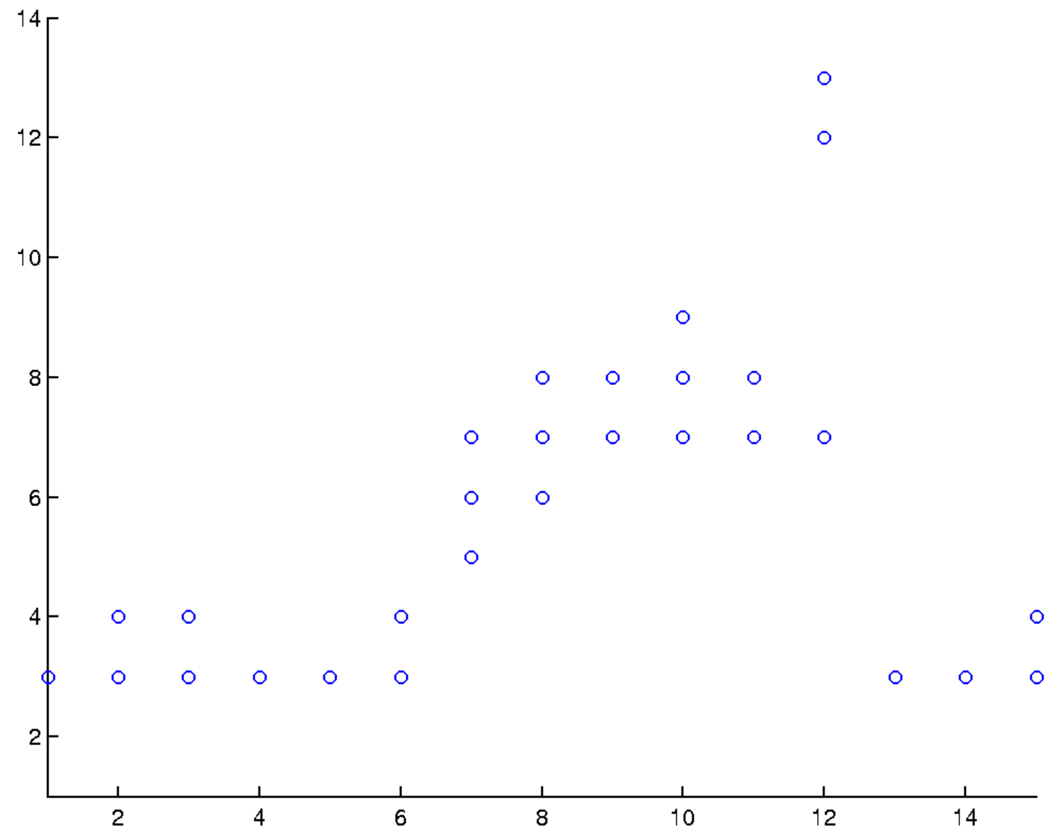
Grid-Sequencing Performance



Time improvement ratios for TRON ($n = 101,761$)

Grid-Sequencing Performance



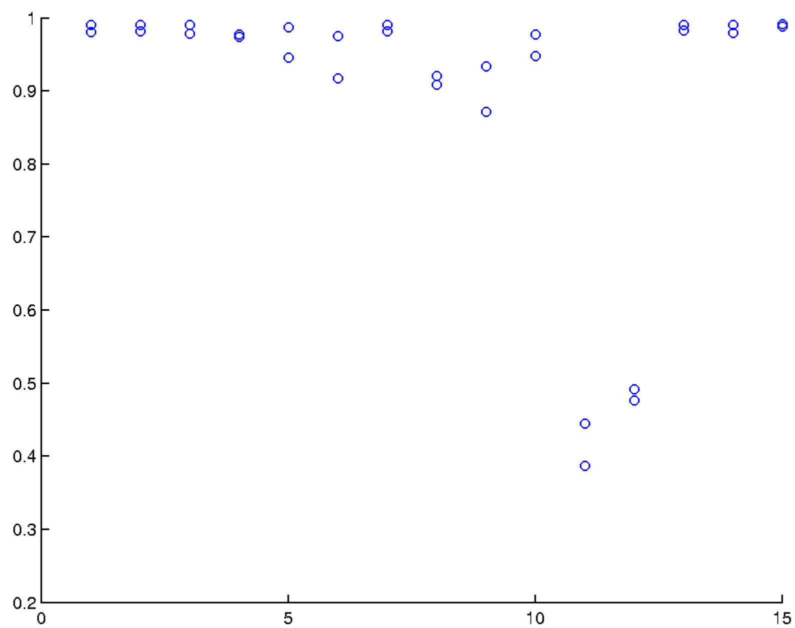
Number of iteration for TRON, levels 5, 6, 7.

Order of convergence for $f(x_h^*)$

The order of convergence is defined as the $p > 0$ such that

$$f(x_h^*) \sim f(x^*) + \alpha h^p, \qquad h \to 0$$

where $h = 1/n$ and n is the number of variables.



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Order of convergence for x_h^*

The order of convergence is defined as the $p > 0$ such that

$$\|x_h^*\|_2 \sim \|x^*\|_2 + \alpha h^p, \qquad h \to 0$$

where $h = 1/n$ and n is the number of variables.